

Off-equilibrium Langevin dynamics of the discrete nonlinear Schrödinger chain

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Abstract. Suitable Langevin thermostats are introduced which are able to control both the temperature and the chemical potential of a one-dimensional lattice of nonlinear Schrödinger oscillators. The resulting non-equilibrium stationary states are then investigated in two limit cases (low temperatures and large particle densities), where the dynamics can be mapped onto that of a coupled-rotor chain with an external torque. As a result, an effective kinetic definition of temperature can be introduced and compared with the general microcanonical (global) definition.

Keywords: Transport processes / heat transfer (Theory)

Submitted to: *Journal of Statistical Mechanics: theory and experiment*

PACS numbers: 63.10.+a 05.60.-k 44.10.+i

1. Introduction

Understanding transport properties in open many-particle systems is one of the main goals of contemporary nonequilibrium statistical mechanics. The ultimate goal is that of finding the statistical measure for stationary out-of-equilibrium conditions. In fact, this would allow evaluating the fluctuations of the relevant macroscopic observables (such as the currents) and, possibly, deriving the corresponding transport equations, without any *ad hoc* statistical assumption. In view of the many technical difficulties that one typically encounters along this path, it is convenient to start investigating simple models, like chains of nonlinear oscillators [1, 2]. A particularly interesting system is the Discrete Nonlinear Schrödinger (DNLS) equation [3, 4] that has important applications in many domains of physics. A classical example is electronic transport in biomolecules [5], while in optics or acoustics it describes the propagation of nonlinear waves in a layered photonic or phononic media [6, 7]. With reference to cold atomic gases, the DNLS equation provides an approximate semiclassical description of bosons trapped in periodic optical lattices (for a recent survey see [8] and references therein).

This system is rather interesting since the presence of two conserved quantities (energy and number of particles) naturally requires arguing about coupled transport, in the sense of ordinary linear irreversible thermodynamics. In fact, in spite of the many studies of heat conduction in oscillator chains [1, 2, 11, 12], coupled transport processes have been scarcely investigated [13, 14, 15, 16, 17]. Furthermore, the DNLS equation has been mostly studied because of the breather solutions that can spontaneously emerge [18], while the analysis of its nonequilibrium properties is still in its early days [9, 10].

The statistical analysis of any system of physical interest requires a proper modelling of the interaction with an external reservoir. The reservoir is expected to exchange energy and particles with the system until a steady state is reached, characterized by the expected temperature and chemical potential. In standard oscillator chains, this is typically achieved by introducing Langevin thermostats (e.g., see [1, 2]). In models like the DNLS equation, this option is less straightforward, because of its peculiar structure and symmetries. In this paper we augment the Hamiltonian equation with a suitable nonlinear damping and a stochastic term to model the interaction with one or more reservoirs. To our knowledge, this is the first such scheme to be proposed in the literature, at least in the present context, although one should mention [19], where the evolution of a DNLS system has been discussed in the presence of small nonlinear damping and a multiplicative noise.

This general Langevin scheme is then used to investigate transport properties in two limit cases, low temperatures and large particle densities, where the DNLS model reduces to a chain of coupled oscillators with just internal forces. In fact, it turns out that norm (number of particles) conservation is mapped onto the conservation of (angular) momentum. Such a relationship helps also to understand the reason why DNLS chains are characterized by a normal [10], rather than anomalous transport, as in typical translationally invariant nonlinear systems [1]. The corresponding oscillators, in fact, involve phase-like variables such as the XY model: in such models, phonons are scattered by the occasional phase-jumps scatter the phonons, thereby contributing to a normal diffusion [1]. Moreover, we find that the chemical potential, which is associated with norm conservation, turns out to be equivalent to the rotation frequency of the single rotors and the corresponding force that must be exerted by the external Langevin reservoir for its thermalization is an additional constant torque. Finally, the possibility to map the DNLS equation onto a standard chain of coupled (phase) oscillators allows deriving a local microscopic definition of the temperature, based on their kinetic energy.

The paper is organized as follows. In section 2 we recall some basic properties of the model at finite-temperature. In section 3 we present the Langevin equations and discuss the equilibrium setup as well as the case of two external reservoirs at different temperatures and chemical potentials. The rest of the paper focuses on two limit cases: we first consider the weakly-nonlinear limit, which can be analysed by introducing a suitable harmonic approximation (section 4), and then pass to the large particle-density limit (section 5), where the dynamics can be mapped onto that of a chain of coupled (nonlinear) rotors. A numerical test on the corresponding definitions of kinetic temperatures is provided in section 6, while section 7 is devoted to a final discussion about the achievements and perspectives of the present study. Finally, the appendix contains an alternative derivation of the generalized Langevin equations.

2. The DNLS model at equilibrium

The isolated one-dimensional DNLS equation, defined (in suitable units) on a lattice of N sites, reads

$$i\dot{z}_n = -2|z_n|^2 z_n - z_{n+1} - z_{n-1} \quad , \quad (1)$$

where the quantity $|z_n|^2$ can be interpreted as the *number of particles*, or, equivalently, the *mass* at site n . Eq. (1) can be derived from the Hamiltonian

$$H = \sum_{n=1}^N (|z_n|^4 + z_n^* z_{n+1} + z_n z_{n+1}^*) \quad . \quad (2)$$

The sign of the quartic term is assumed to be positive, i.e. we consider the case of repulsive on-site interaction; the sign of the hopping term is irrelevant, due to the symmetry associated with the canonical (gauge) transformation $z_n \rightarrow z_n e^{i\pi n}$. With this choice of the sign of the nonlinear term and assuming periodic boundary conditions, the ground state of the isolated chain is the time periodic solution $z_n = \sqrt{a} e^{i[\omega t + \pi n]}$, where the parameter a fixes the value of the mass density, with $\omega = 2(a - 1)$ [20].

The equilibrium statistical mechanics of the continuous nonlinear Schrödinger equation was first studied in [21], while that of its discrete, nonintegrable, version (1) was developed more recently in [20]. Several conclusions of these studies have been extended to a wider class of nonlinear lattices, whose dynamics is described by DNLS-like equations [22].

An important property of the DNLS dynamics is that it conserves two quantities, the energy (2) and the total mass

$$A = \sum_{n=1}^N |z_n|^2 = \frac{1}{2} \sum_{n=1}^N (p_n^2 + q_n^2) \quad , \quad (3)$$

where we have introduced, for later reference, the notations $z_n \equiv (p_n + iq_n)/\sqrt{2}$. As a consequence, the equilibrium phase-diagram is two-dimensional, as it involves the energy density $h = H/N$ and the mass density $a = A/N$ (in a microcanonical description of thermodynamic equilibrium) or, equivalently the temperature T and the chemical potential μ (in a grand-canonical description of thermodynamic equilibrium). The first reconstruction of the equilibrium phase-diagram was reported in [20] for the grand-canonical ensemble, with the help of transfer integral techniques. For our purposes, it is sufficient to recall that the positive-temperature states are located in the region of the (a, h) plane lying between the ground-state line (see Fig. 1)

$$h = a^2 - 2a \quad T = 0, \quad \mu = 2(a - 1)$$

and the infinite-temperature one (corresponding to random phases)

$$h = 2a^2 \quad T = \infty, \quad \mu = -\infty \quad . \quad (4)$$

Above the $T = \infty$ line, one finds the so-called negative-temperature states [20]. In this region, the dynamics of the DNLS equation is characterized by long-lived localized excitations (discrete breathers) [23]. Its thermodynamic properties will not be considered here: we refer to [24] and to the literature cited therein for an account on the role of these peculiar states on the equilibrium properties of the DNLS equation. The nonequilibrium studies discussed in this paper all refer to the positive-temperature region.

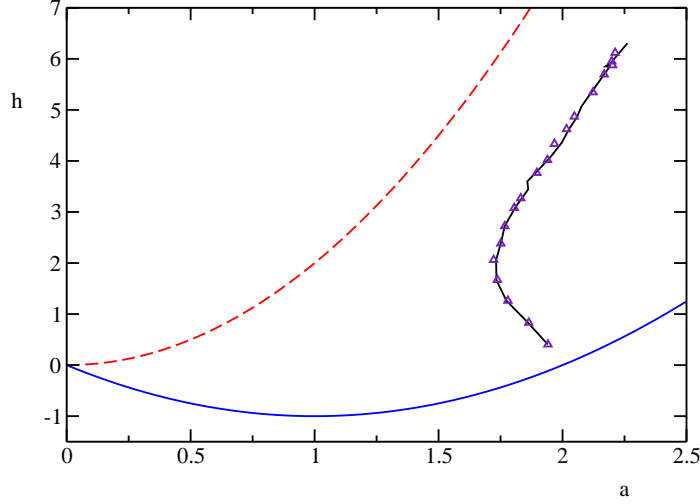


Figure 1. Equilibrium phase diagram of the DNLS model in the (a, h) plane. The positive temperature region lies between the ground state (solid blue line) and the infinite temperature isothermal (dashed red line). The line at constant chemical potential $\mu = 2$ has been reconstructed using the Monte-Carlo stochastic thermostats [10] (purple triangles) and the Langevin scheme (solid black line).

3. Langevin thermostats

Being interested in exploring the thermodynamic properties of a Hamiltonian system, the first problem we have to deal with is that of introducing suitable thermal baths. In separable Hamiltonian systems (i.e., those composed of a kinetic and a potential energy) it is sufficient to modify the momentum equation, by adding a linear dissipation term of the type $-\gamma p_i$ accompanied by a white-noise fluctuation, whose amplitude determines the value of the temperature. This simple Langevin-like scheme does not work for the DNLS. In fact, one can easily check that in the absence of fluctuations (i.e. in the zero-temperature limit) this dissipative dynamics indeed converges to a fixed point, that does not correspond to the ground state, which, as mentioned in the previous section, is a time-periodic solution [20].

The problem can be overcome by adopting the following scheme,

$$i\dot{z}_n = (1 + i\gamma) [-2|z_n|^2 z_n - z_{n+1} - z_{n-1}] + i\gamma\mu z_n + \sqrt{\gamma T} \xi_n(t) \quad , \quad (5)$$

where $\xi_n(t) = \xi'_n + i\xi''_n$ is a complex, Gaussian, white random noise with unit variance. In practice, the above equation corresponds to a series of thermostats all operating at temperature T and chemical potential μ , and with the same coupling strength γ to the single DNLS degrees of freedom. This is basically a stochastic, discrete, complex Ginzburg-Landau equation. As required for a meaningful reservoir, the dissipative term vanishes for the ground state evolution, $z_n = \sqrt{a} \exp[i(\omega t + \pi n)]$.

In the Appendix we show that the Langevin scheme in Eq. (5) can be interpreted (with the help of suitable assumptions and approximations) as the action of an ensemble of linear oscillators. Some physical insight can be, however, gained by simply rewriting Eq. (5), in terms of the p_n q_n variables,

$$\dot{p}_n = -(p_n^2 + q_n^2)q_n - q_{n+1} - q_{n-1} - \gamma \frac{\partial H_\mu}{\partial p_n} + \sqrt{2\gamma T} \xi'_n(t) \quad (6)$$

$$\dot{q}_n = (p_n^2 + q_n^2)p_n + p_{n+1} + p_{n-1} - \gamma \frac{\partial H_\mu}{\partial q_n} + \sqrt{2\gamma T} \xi_n''(t) \quad ,$$

where and H_μ is the effective Hamiltonian $H_\mu = H - \mu A$. The two deterministic terms, proportional to γ in the r.h.s. of the above equations, are gradient terms: in the absence of the symplectic component, they would drive the system towards a time-independent state with a minimal H_μ . On the other hand, the addition of the symplectic forces ensures a (periodic) motion across the microstates characterized by the same H_μ value. Accordingly, it is reasonable to conclude that this is the proper way to including a dissipation scheme in the DNLS case. The reason why H_μ is considered instead of H is the presence of two conservation laws: the minimum of the energy depends on the mass density a that has to be, on the average, preserved and this can be achieved by adding the term $-\mu A$ into the effective Hamiltonian, where μ plays the role of the chemical potential. The additional presence of the fluctuation terms completes the definition of the generalized Langevin equation, that describes the coupling of the DNLS chain with a proper stochastic reservoir with temperature T and chemical potential μ .

The Langevin equations (6) can be straightforwardly generalized to a non-equilibrium setting, by assuming that the single reservoirs operate at different temperatures/chemical potentials. In the following we will focus on a typical setup in which only the first (z_1) and the last (z_N) lattice variables interact with the reservoirs. This means that, assuming fixed boundary conditions (i.e. $z_0 = 0$), the evolution on the leftmost site is rule by the equation

$$\begin{aligned} \dot{p}_1 &= -(p_1^2 + q_1^2)q_1 - q_2 - \gamma [(p_1^2 + q_1^2)p_1 + p_2 - \mu_L p_1] + \sqrt{2\gamma T_L} \xi_1' \\ \dot{q}_1 &= (p_1^2 + q_1^2)p_1 + p_2 - \gamma [(p_1^2 + q_1^2)q_1 + q_2 - \mu_L q_1] + \sqrt{2\gamma T_L} \xi_1'' \quad , \end{aligned} \quad (7)$$

where T_L and μ_L denote the temperature and the chemical potential of the left reservoir, respectively. Analogous equations hold for the right reservoir, which acts on the site $n = N$, where the temperature is T_R , the chemical potential is μ_R , and the coupling strength again equal to γ . The rest of the chain follows the Hamiltonian evolution (1). In order to test the correctness of the method, we have first simulated a chain in contact with two reservoirs operating at the same temperature and chemical potential. In Fig. 1, we compare the isochemical line $\mu = \text{const}$, determined from the Langevin dynamics (7), with the result with a Monte Carlo thermostat, as the one described in [10]. The agreement is well within the statistical fluctuations. Moreover, in Fig. 2 we show a typical relaxation process towards an equilibrium state characterized by the temperature and the chemical potential imposed by the reservoir. In fact, the inset in the same figure shows that the asymptotic state is spatially homogeneous as revealed by the flat mass and energy density profiles.

Although the focus of this paper is on low-temperature transport, it is instructive to analyze first the limit of large temperatures. In separable Hamiltonian models, large temperatures necessarily correspond to large momenta and large fluctuations of the displacement variables. In the DNLS case such conditions occur only if also the chemical potential μ is sufficiently large. In this limit, in order to avoid that the Hamiltonian dynamics is washed out by the fluctuations, it is necessary to assume a vanishing dissipation. In the limit $T \rightarrow \infty$, $\mu \rightarrow -\infty$ (stability is ensured only for negative values of μ) and $\gamma \rightarrow 0$, Eq. (5) simplifies to

$$i\dot{z}_1 = -2|z_1|^2 z_1 - z_2 + i\gamma\mu_L z_1 + \sqrt{\gamma T_L} \xi_1 \quad . \quad (8)$$

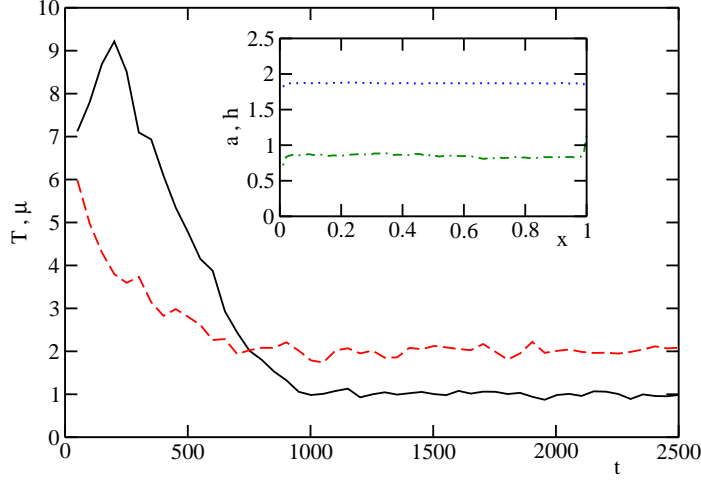


Figure 2. Evolution of T (black solid line) and μ (red dashed line) in a chain of $N = 100$ sites in contact with two Langevin heat baths with $T_L = T_R = 1$, $\mu_L = \mu_R = 2$. The initial state corresponds to $a = 4$ and $h = 15$. T and μ are measured according to [10] and averaged over running windows of 50 time units. In the inset: final spatial profiles of mass (blue dots) and energy (green dot-dashed line) densities as a function of the rescaled site index $x = n/N$.

Upon introducing $\Gamma = -\gamma\mu_L > 0$ and $a_L = -T_L/\mu_L$, this equation can be written as

$$i\dot{z}_1 = -2|z_1|^2 z_1 - z_2 - i\Gamma z_1 + \sqrt{a_L\Gamma} \xi_1 \quad . \quad (9)$$

This is the “naive” DNLS Langevin equation, which thus we see it corresponds to the infinite temperature limit, i.e. it simulates only the points located along the line defined by Eq. (4). In Fig. 3 we show that this holds true also in the nonequilibrium setting, when a_L is assumed to be different from a_R . In the steady state, the energy and density profiles fulfill the relation (4) at any point of the chain. Moreover, we have checked that the distribution of the local mass is Poissonian, as expected in the $T = \infty$ case [23] (see the inset of Fig. 3) .

4. The low-temperature limit

In order to explore the low-temperature limit, it is useful to express the solution of the dynamics (1) as

$$z_n = Z(1 + \zeta_n) \exp[i(\omega t + \phi_n + n\pi)] \quad . \quad (10)$$

Notice that the ground state solution corresponds to $\zeta_n = 0$ and $\phi_n = 0$ with $Z = \sqrt{a}$ and $\omega = 2(Z^2 - 1)$.

By inserting (10) into Eq. (1), one finds that the new variables ζ_n and ϕ_n obey the following dynamical equations

$$\begin{aligned} \dot{\phi}_n(1 + \zeta_n) &= 2B\zeta_n + 2Z^2(3\zeta_n^2 + \zeta_n^3) - (1 + \zeta_{n+1}) \cos(\phi_{n+1} - \phi_n) \\ &\quad - (1 + \zeta_{n-1}) \cos(\phi_n - \phi_{n-1}) + 2 \\ \dot{\zeta}_n &= (1 + \zeta_{n+1}) \sin(\phi_{n+1} - \phi_n) - (1 + \zeta_{n-1}) \sin(\phi_n - \phi_{n-1}) \quad , \end{aligned} \quad (11)$$

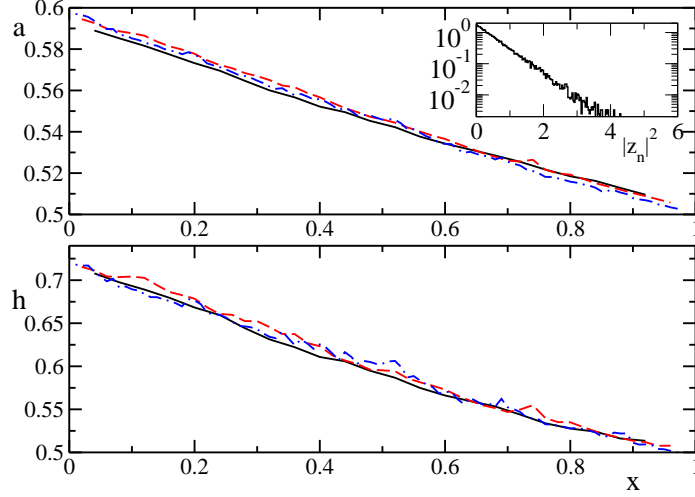


Figure 3. Nonequilibrium profiles of mass density (upper panel) and energy density (lower panel) obtained with the infinite temperature Langevin equation (9) and parameters $a_L = 0.6$, $a_R = 0.5$, $\Gamma = 1$. Black solid, red dashed and blue dot-dashed lines refer respectively to chain lengths $N = 25, 50, 100$. The profiles are almost linear and $h(x) = 2a^2(x)$ along the chain, confirming that the thermostats act at $T = \infty$. The inset shows that histogram of the local mass $|z_n|^2$ at $n = 20$ is Poissonian, as expected.

where $B = 1 + 2Z^2$. In the low-temperature limit, the solution of these equations is expected to be close to the homogeneous periodic motion of the ground-state solution. Thus, we can assume that $\zeta_n \ll 1$ and $(\phi_n - \phi_{n-1}) \ll 1$. As a result, Eq. (11) simplifies to

$$\begin{aligned} \dot{\phi}_n &= 2B\zeta_n - \zeta_{n+1} - \zeta_{n-1} \\ \dot{\zeta}_n &= (\phi_{n+1} - 2\phi_n + \phi_{n-1}) \end{aligned} \quad (12)$$

If one now introduces the new variable

$$p_n = 2B\zeta_n - \zeta_{n+1} - \zeta_{n-1} \quad (13)$$

the Eqs. (12) can be re-written as

$$\begin{aligned} \dot{\phi}_n &= p_n \\ \dot{p}_n &= 2(1+B)(\phi_{n+1} - 2\phi_n + \phi_{n-1}) - \phi_{n+2} + 2\phi_n - \phi_{n-2} \end{aligned} \quad (14)$$

These equations describe the dynamics of a chain of harmonic oscillators with nearest-neighbour and next-to-nearest-neighbour. The corresponding Hamiltonian,

$$\mathcal{H}_h = \sum_n \left[\frac{1}{2} p_n^2 + (1+B)(\phi_{n+1} - \phi_n)^2 - \frac{1}{2}(\phi_{n+2} - \phi_n)^2 \right] \quad (15)$$

is, at leading order in p_i and $(\phi_{n+1} - \phi_n)$, fully equivalent to that of the original DNLS equation. Its quadratic structure is hardly a surprise, since it essentially originates from a parabolic approximation around the minimum of the energy. The normal modes, i.e. the plane-wave solutions of Eqs. (14), are the discrete analogs of the Bogoliubov modes, in the context of the physics of atomic condensates [26].

Passing to thermodynamics, a first interesting implication of the Hamiltonian structure in the low-temperature limit is that one can naturally introduce a microscopic definition of temperature as the average kinetic energy, i.e.

$$T_h = J \langle (2B\zeta_n - \zeta_{n+1} + \zeta_{n-1})^2 \rangle, \quad (16)$$

where the proportionality constant J is the Jacobian determinant of transformation (13), which must be included to allow for a meaningful comparison with the DNLS model. We have measured T_h by numerical simulations of the Langevin scheme defined in Eq. (5) and in Fig. 4 we have compared it with the temperature of the bath, $T_B \equiv T_L = T_R$, for different values of the mass density, a . As expected, T_h approaches T_B for increasing values of a . In fact, the larger is a , the smaller is the relative amplitude of the fluctuations with respect to the ground state.

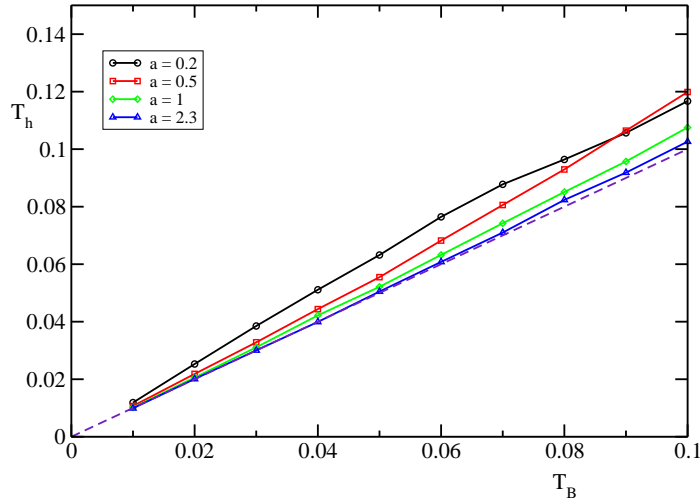


Figure 4. Comparison of the harmonic temperature T_h , Eq. (16) with the reservoir temperature, T_B . The dashed line correspond to $T_h = T_B$. The Langevin heat baths are coupled at the boundaries of a DNLS chain with $N = 50$. T_h is measured on a subchain of 30 lattice sites to increase the statistics. The values of the Jacobian determinant J , which are the product of the eigenvalues of a tridiagonal matrix, have been computed analytically in the $N \rightarrow \infty$ limit and are $J = 5.95, 3.73, 2.91, 2.42$ for curves from top to bottom.

Altogether, the original DNLS equation in the low-temperature limit maps onto a translationally invariant harmonic chain with nearest- and next-to-nearest-neighbour interactions (the former being attractive and the latter repulsive). Moreover, the total mass-conservation law of the DNLS maps onto the conservation of the total momentum $P = \sum p_n$. The harmonic structure of Hamiltonian (15) implies that the dynamics can be decomposed into that of non-interacting phonons. As a result, for what concerns transport properties, in the low-temperature regime, the heat conductivity should exhibit a divergence in the thermodynamic limit, as expected for any harmonic (integrable) model (see [27, 1]). On the other hand, previous non-equilibrium studies of the DNLS model have revealed that the heat conductivity is finite [10] at finite temperatures. This is clearly a consequence of the nonlinear terms which break the integrability of the dynamics. However, it is not obvious how this can happen in a translationally invariant model such as (15), since it is known that in the absence of

pinning forces, the heat conductivity diverges in the thermodynamic limit [1, 11]. The problem is solved in the next section, where we discuss the tight relationship with the one-dimensional XY model.

5. Large mass-densities

Another interesting limit of the DNLS model is that of large a values, that is equivalent to small-amplitude fluctuations. This limit can be analyzed by applying a different perturbative scheme, which allows preserving relevant nonlinear terms, thus yielding more meaningful predictions. The starting point is again Eq. (11), where we assume $Z \gg 1$ and $\zeta_n \approx \mathcal{O}(1)$. The dynamical equations (1) simplify to

$$\begin{aligned}\dot{\phi}_n &= 2Z^2\zeta_n(2 + 3\zeta_n^2 + \zeta_n^3)/(1 + \zeta_n) \\ \dot{\zeta}_n &= (1 + \zeta_{n+1})\sin(\phi_{n+1} - \phi_n) - (1 + \zeta_{n-1})\sin(\phi_n - \phi_{n-1})\end{aligned}\quad (17)$$

It is not clear whether these equations may describe a Hamiltonian dynamics (in fact, ϕ_n and ζ_n are not canonical variables). If, however, we introduce the additional assumption $\zeta_n \ll 1$ and rescale ζ_n to $\lambda_n = 4Z^2\zeta_n$, we obtain, to leading order,

$$\begin{aligned}\dot{\phi}_n &= \lambda_n \\ \dot{\lambda}_n &= 4Z^2[\sin(\phi_{n+1} - \phi_n) - \sin(\phi_n - \phi_{n-1})]\end{aligned}\quad (18)$$

which corresponds to a system of coupled rotors, i.e. a classical version of the XY model in one dimension [28, 29, 30, 31], with Hamiltonian

$$\mathcal{H}_{XY} = \sum_n \frac{\lambda_n^2}{2} - \sum_n 4Z^2 \cos(\phi_{n+1} - \phi_n) \quad , \quad (19)$$

where λ_n and ϕ_n act as a couple of conjugated action-angle variables, the former playing the role of an angular momentum. This analogy was already noticed in a 2d setup in [32]. At variance with the previous section, we have not introduced any smallness hypothesis for $\phi_n - \phi_{n-1}$; this is the reason why some nonlinear terms have been kept.

The XY Hamiltonian (19) can be obtained more rigorously by applying a sequence of canonical transformations to the original DNLS model. Let us first introduce the transformation to action-angle variables $z_n = \sqrt{a_n} \exp[i(\omega t + \phi_n + n\pi)]$ and re-write the DNLS Hamiltonian (2) in the form

$$H = \sum_n a_n^2 - 2\sqrt{a_n a_{n+1}} \cos(\phi_{n+1} - \phi_n) - \omega a_n \quad , \quad (20)$$

where the last term in the Hamiltonian follows from the time-dependence of the transformation. Taking inspiration from the procedure discussed in the previous section, one could then set $a_n = Z^2(1 + \zeta_n)^2$. This transformation is, however, not canonical and this is the reason why Eqs. (17) are not symplectic. One can, nevertheless, proceed by defining $a_n = Z^2 + 2Z^2\zeta_n$, a (linear) canonical transformation, which approximates better and better the previous expression for increasing values of Z . By then recalling that $\omega = 2(Z^2 - 1)$ and expanding in Z , the Hamiltonian (19) is finally obtained, up to an irrelevant constant shift.

It is interesting to observe that in this large-density limit the invariance under rotation of the DNLS transforms into the invariance under a translation of the angles ϕ_n . Accordingly, the conservation of the total mass A transforms into the conservation of the total angular momentum $L = \sum_n \lambda_n$ (this can be easily verified by expanding

the expression of the total mass). This analogy provides an interesting interpretation of the chemical potential μ . In fact, the Boltzmann weight for a system rotating with an angular momentum L and average frequency ω is $\exp\{-\beta[H - \omega L]\}$, to be compared with the DNLS grand-canonical weight $\exp\{-\beta[H - \mu A]\}$, thus yielding the identification of ω with μ .

Before passing to thermodynamic studies, it is necessary to comment about the range of validity of the XY model as an approximation of the DNLS one. The condition $\zeta_n \ll 1$ implies $\lambda_n \ll Z^2 = a$, i.e. $T \ll a^2$, because on average λ_n^2 is equal to the temperature T . As we are exploring the range of large values of $Z = \sqrt{a}$, one can conclude that, the larger Z , the broader the temperature range where the XY model provides an accurate description of the DNLS equation. Before drawing this conclusion, it is, however, necessary to be more careful. In fact, the presence of a finite conductivity in the XY model can be traced back to the existence of (possibly infrequent) jumps of angle-differences across the sinusoidal potential barrier. In the context of Eq. (19), the height of this barrier is of the order of $Z^2 = a$ which is smaller than the maximal acceptable energy a^2 (since $a \ll a^2$, for $a \gg 1$). More than that, the validity of the XY model extends to the high-temperature regime (here “high” means above a) characterized by frequent jumps.

Finally, we compare Hamiltonians (15) and (19). The former one is valid in the low-temperature regime, while the latter applies for $Z \gg 1$ (and $T \ll a^2$). Accordingly, they should reduce to one another for small T and large Z . This is indeed the case, because the next-to-nearest-neighbour interaction in (15) is negligible for $Z \gg 1$ and, in the low-temperature limit, one can expand the cosine interaction in (19) around zero.

5.1. Thermostatted chain

Here, we study a DNLS chain in contact with external Langevin reservoirs in the large mass-density limit. It is convenient to introduce the chemical-potential difference $\delta\mu = (\mu_L - \mu_R)/2$ and its average value $\mu = (\mu_L + \mu_R)/2 = 2(Z^2 - 1)$. From Eq. (7), we find that (for the sake of simplicity we write the evolution equation for the leftmost side),

$$i\dot{z}_1 = -2|z_1|^2 z_1 - z_2 - i\gamma [2|z_1|^2 z_1 + z_2 - (2Z^2 - 2)z_1 - \delta\mu z_1] + \sqrt{\gamma T_L} \xi_1. \quad (21)$$

If we assume $Z \gg 1$ and a small dissipation γ , namely

$$\gamma = \frac{\gamma'}{4Z^2}, \quad (22)$$

where γ' is of order ∞ , we can transform the previous equation into those for the XY model, with suitable dissipation and fluctuation terms

$$\begin{aligned} \dot{\phi}_1 &= 4Z^2 \zeta_1 \\ \dot{\zeta}_1 &= \sin(\phi_2 - \phi_1) - \gamma' \left(\zeta_1 - \frac{\delta\mu}{4Z^2} \right) + \frac{\sqrt{\gamma' T_L}}{2Z^2} \xi_1, \end{aligned} \quad (23)$$

where we have neglected the nonlocal dissipation z_2 and another term proportional to ζ_1 , as they are both negligible in this limit. By turning to the above defined rescaled momenta λ_n , we obtain

$$\begin{aligned} \dot{\phi}_1 &= \lambda_1 \\ \dot{\lambda}_1 &= 4Z^2 \sin(\phi_2 - \phi_1) - \gamma' (\lambda_1 - \delta\mu) + \sqrt{4\gamma' T_L} \xi_1. \end{aligned} \quad (24)$$

The equations for the rightmost site of the chain are the same as the above except for $\delta\mu$ and T_L that are replaced by $-\delta\mu$ and T_R , respectively. Notice that the chemical-potential-differences $\pm\delta\mu$ applied at the boundaries of the DNLS chain correspond to constant torques $\pm\gamma'\delta\mu$ (i.e. a sort of external pressure) for the XY model.

Eq. (24) without external torque and noise has been investigated in [33]. A closer version of the model (24) has been studied by Olla et al. [34], who, however, have introduced the constant-force term without relating it to the presence of the external bath. As a result, the external forcing does not vanish in the small coupling limit, with some weird physical implications for the microcanonical simulations due to the possible occurrence of an unbounded acceleration (if $\delta\mu$ is large enough).

5.2. Fluxes

The continuity equations for mass and energy densities allow determining explicit expressions for the corresponding fluxes,

$$j_n^a = i(z_n z_{n-1}^* - z_n^* z_{n-1}) \quad (25)$$

$$j_n^h = \dot{z}_n z_{n-1}^* + \dot{z}_n^* z_{n-1} \quad (26)$$

In the large-mass limit, the leading terms read

$$j_n^a = -2Z^2 \sin(\phi_{n+1} - \phi_n) \quad (27)$$

$$j_n^h = -2\omega Z^2 \sin(\phi_{n+1} - \phi_n) - 4Z^2 \dot{\phi}_n \sin(\phi_{n+1} - \phi_n) \quad , \quad (28)$$

where the variables ζ_n have been expressed in terms of ϕ_n . Notice that the simple symmetric form of the second equation has been obtained by adding to (26) the quantity $-Z^2(\dot{\phi}_n - \dot{\phi}_{n-1})\sin(\phi_n - \phi_{n-1})$, whose average is zero in a stationary state. Eq. (27) is just the momentum flux of the XY model, i.e. its local force. The term proportional to $\dot{\phi}_n$ in Eq. (28) has the typical structure of the energy flux in the XY model: it is nonzero only at finite temperatures. The first term is a coherent contribution that results from the fact that the oscillators rotate with an average common frequency ω : it survives in the zero-temperature limit, when $j_n^h = \mu j_n^a$, so that the heat current $j_n^h - \mu j_n^a = 0$, i.e. there is no heat transport and no entropy production. At low temperatures, Eqs. (27,28) describe the Josephson effect, where the chain amounts to a single junction in between two superfluids [26]. The mass current is proportional to the phase gradient and is independent of the system length N , i.e. it provides a ballistic contribution.

6. Comparison with numerical simulations

An important difference between the DNLS equation and oscillator chains (like the Fermi-Pasta-Ulam or Klein-Gordon models) is that its Hamiltonian is not the sum of kinetic and potential energies. Therefore, it is not obvious how to directly monitor the temperature T and the chemical potential μ in actual simulations. The only general approach we are aware of is based on non-local microcanonical expressions [35],[10]) which, at least require averaging over small subchains (see [10] for details).

On the other hand, the DNLS/XY correspondence provides an effective definition of temperature. In fact, from (19) it is straightforward to define a kinetic temperature in the standard way

$$T_{XY} = \langle \lambda_n^2 \rangle \quad (29)$$

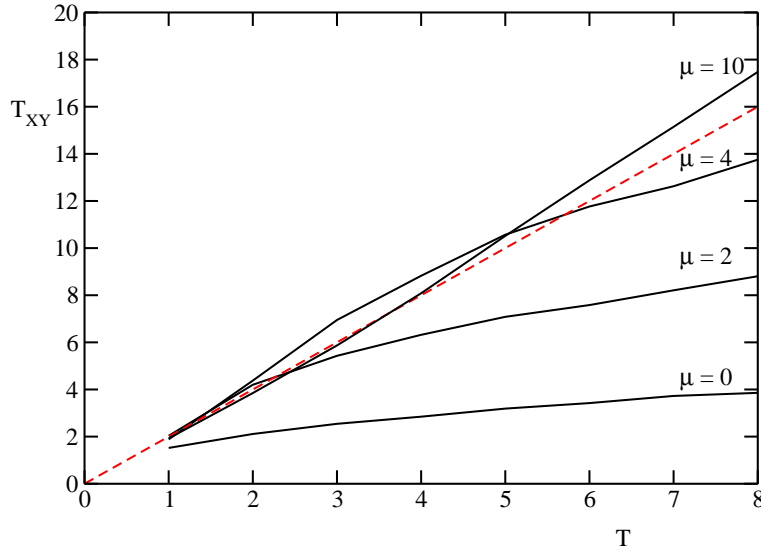


Figure 5. Comparison of the XY kinetic temperature T_{XY} with T . Simulations are performed using Langevin heat baths. The dashed line correspond to $T_{XY} = 2T$, which should hold in the limit of large μ , where the XY approximation is valid. The heat baths are coupled at the boundaries of a DNLS chain with $N = 50$. T_{XY} and T are measured on a subchain of 30 lattice sites.

One can easily check that in the limit of large Z , the kinetic temperature T_h , defined in (16), reduces to (29). Furthermore, if we compare the stochastic term in Eq. (24) with the one imposed by the fluctuation-dissipation theorem and commonly used in the Langevin equation for oscillator models, $\sqrt{2\gamma T}$ (see [1, 2]), we can conclude that our definitions imply $T_{XY} = 2T$ (the factor 2 is just a consequence of the choice of the transformation of variables, and has the same origin as the proportionality factor J in (16)).

In Figure 5 we compare T , defined as in [10], with T_{XY} for an equilibrium setting, i.e. external reservoirs at equal temperature. T_{XY} is computed by evaluating, in the same simulation, the average of the ζ_n^2 defined in (10). The data clearly show that, by increasing the chemical potential μ (i.e., by increasing Z), the range of values in which the two temperatures coincide increases, as expected from the previous considerations.

Finally, we have tested the validity of the XY approximation in a non-equilibrium stationary regime, by imposing a temperature difference ΔT and a small chemical potential difference $\delta\mu$ with respect to a reference equilibrium state (T, μ) , where the XY approximation holds. As expected, Fig. 6 exhibits a nice agreement between the two definitions of the temperature profiles. A further test of the validity of XY model is presented in Table 1 where the full DNLS fluxes are compared with the ones reconstructed through the XY approximation (see Eqs. (27)).

7. Conclusions

In this paper, we have introduced suitable stochastic heat baths which can control both the temperature and the chemical potential in a DNLS model. At variance

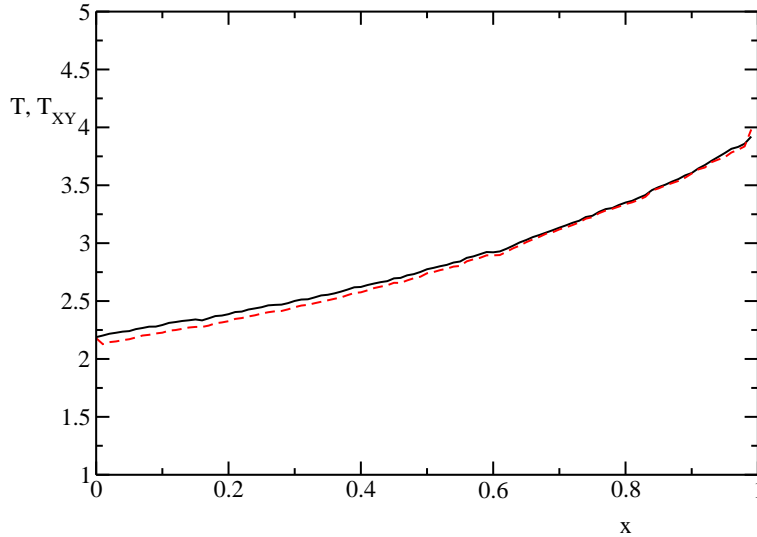


Figure 6. Comparison of the XY kinetic temperature profile T_{XY} (red dashed line) with T [10] (black solid line) in a nonequilibrium steady state. Simulations are performed using Langevin heat baths with parameters $(T_L = 2, \mu_L = 9.6)$ and $(T_R = 4, \mu_R = 10.4)$.

	DNLS	XY
\dot{j}_a	-0.234	-0.208
\dot{j}_h	-1.40	-1.28

Table 1. Comparison of the exact DNLS fluxes (first column) and the ones reconstructed by means of eqs.(27) (second column) for the nonequilibrium profile described in the caption of Fig. 6.

with the Monte Carlo dynamics [10], the Langevin equation allows establishing direct relationships with standard chains of oscillators. In the low-temperature limit, we obtain a quadratic approximation which allows describing the transport through the thermalization of linear excitations (the Bogoliubov modes), in the same spirit as harmonic oscillators in interaction with Langevin baths [27]. In the large mass-density limit, the relevant contribution to the DNLS evolution is due to the phase dynamics, which is described by a suitable XY model in contact with standard Langevin heat baths and an additional external torque. The corresponding energy flux turns out to be the sum of two different contributions, one due to the phase gradient associated with the torque, the other due to angular-velocity fluctuations. This indicates that transport in this region has an almost ballistic component, in agreement with previous observations [10].

The two approximations are useful also because they allow introducing simple kinetic expressions for the temperature, that can safely replace the microcanonical definition. This is of practical importance, considering that the microscopic definitions of T and μ are pretty much involved for a non separable Hamiltonian, like the DNLS one [35].

An obvious extension of the present work would be to consider the DNLS model

on two-dimensional lattices. In this case, the correspondence with the XY model would predict the possibility of observing the transition from normal to anomalous behavior of transport coefficients at the Kosterlitz-Thouless-Berezinskii transition [36, 37].

Acknowledgments

We thank S. Olla and Y. Dubi for fruitful discussions.

Appendix: Derivation of the Langevin equation

In this appendix we derive Eq. (5) by following the system-bath coupling approach [38]. In analogy with what done for harmonic lattices [39], we consider a complex oscillator, described by the dynamical variable z , linearly coupled with a bath of independent, complex harmonic oscillators described by the Hamiltonian

$$H_B = \sum_{\nu} \{ \omega_{\nu}^a |a_{\nu}|^2 + \omega_{\nu}^b |b_{\nu}|^2 + [K_{\nu}^* z (a_{\nu}^* + b_{\nu}) + c.c.] \} \quad , \quad (30)$$

where we have introduced two different species of oscillators, corresponding to the two sets of frequencies ω_{ν}^a and ω_{ν}^b , while K_{ν} are the bath-system coupling constants. In order to preserve the global symmetry of the system with respect to phase transformations, we impose a second conservation law,

$$A_B = \sum_{\nu} (|a_{\nu}|^2 - |b_{\nu}|^2) \quad . \quad (31)$$

The function A_B is the generator of phase transformations of the bath variables. It is easy to verify that the transformation generated by $A_B + |z|^2$,

$$\begin{aligned} a_{\nu}(s) &= e^{is} a_{\nu}(0) \\ b_{\nu}(s) &= e^{-is} b_{\nu}(0) \\ z(s) &= e^{is} z(0) \quad , \end{aligned}$$

leaves the Hamiltonian H_B invariant. An example of heat bath satisfying these conditions is given by a complex d'Alembert equation, $\square\phi(x, t) = 0$, for which the quantity A_B represents the total (conserved) charge of the field. The equations of motion generated by (30) are

$$\begin{aligned} i\dot{a}_{\nu} &= -\omega_{\nu}^a a_{\nu} - K_{\nu}^* z \\ i\dot{b}_{\nu} &= -\omega_{\nu}^b b_{\nu} - K_{\nu} z^* \\ i\dot{z} &= f(z) - \sum_{\nu} K_{\nu} (a_{\nu} + b_{\nu}^*) \quad , \end{aligned}$$

where $f(z)$ accounts for the deterministic part of the evolution of z , not included in H_B . The first two equations can be formally solved, yielding

$$\begin{aligned} a_{\nu}(t) &= a_{\nu}(0) e^{i\omega_{\nu}^a t} + iK_{\nu}^* \int_0^t e^{i\omega_{\nu}^a(t-t')} z(t') dt' \\ b_{\nu}(t) &= b_{\nu}(0) e^{i\omega_{\nu}^b t} + iK_{\nu} \int_0^t e^{i\omega_{\nu}^b(t-t')} z^*(t') dt' . \end{aligned}$$

By then substituting into the equation for z , we obtain

$$i\dot{z} = f(z) - i \int_0^t G(t-s) z(s) ds + F(t) \quad ,$$

where the noise term $F(t)$ and the dissipation function $G(t)$ are defined as

$$F(t) = - \sum_{\nu} K_{\nu} \left[a_{\nu}(0) e^{i\omega_{\nu}^a t} + b_{\nu}^*(0) e^{-i\omega_{\nu}^b t} \right] \quad (32)$$

$$G(t) = \sum_{\nu} |K_{\nu}|^2 \left[e^{i\omega_{\nu}^a t} - e^{-i\omega_{\nu}^b t} \right] \quad . \quad (33)$$

By now imposing a gran-canonical equilibrium distribution $P \sim \exp[-\beta(H_B - \mu A_B)]$ for the bath of oscillators (where $\beta = 1/T$ is the inverse temperature) [23], we find that the correlation functions of $F(t)$ read

$$\begin{aligned} \langle F(t)F(t') \rangle &= \langle F^*(t)F^*(t') \rangle = 0 \\ \langle F(t)F^*(t') \rangle &= \sum_{\nu} |K_{\nu}|^2 \left[e^{i\omega_{\nu}^a(t-t')} \langle |a_{\nu}(0)|^2 \rangle + e^{-i\omega_{\nu}^b(t-t')} \langle |b_{\nu}(0)|^2 \rangle \right] = \\ &= \sum_{\nu} |K_{\nu}|^2 \left[\frac{e^{i\omega_{\nu}^a(t-t')}}{\beta(\omega_{\nu}^a - \mu)} + \frac{e^{-i\omega_{\nu}^b(t-t')}}{\beta(\omega_{\nu}^b + \mu)} \right] , \end{aligned} \quad (34)$$

where, in order to have positive definite statistical weights, we have also to assume $\omega_{\nu}^a > \mu$ and $\omega_{\nu}^b > -\mu$. In the thermodynamic limit the sums over the index ν in (33) can be replaced by integrals. Accordingly, we can rewrite Eq. (33) in the form

$$G(t) = \int_{\mu}^{+\infty} d\omega G^a(\omega) e^{i\omega t} - \int_{-\mu}^{+\infty} d\omega G^b(\omega) e^{-i\omega t} \quad , \quad (35)$$

where $G^{a,b}(\omega) = \rho^{a,b}(\omega)|K(\omega)|^2$ are two positive definite functions and $\rho^{a,b}(\omega)$ the corresponding density of states that we assume to be smooth functions. By following the same approach, Eq. (34) writes

$$\langle F(t)F^*(t') \rangle = \int_{\mu}^{+\infty} d\omega \frac{G^a(\omega) e^{i\omega(t-t')}}{\beta(\omega - \mu)} + \int_{-\mu}^{+\infty} d\omega \frac{G^b(\omega) e^{-i\omega(t-t')}}{\beta(\omega + \mu)} \quad , \quad (36)$$

which is a kind of fluctuation-dissipation theorem [39] where the Bose-Einstein distribution has been replaced by the Rayleigh-Jeans one.

The corresponding generalized Langevin equation is not very practical, since it is non Markovian. We have nevertheless the freedom to choose the coupling and the density of states of the bath. The spectral properties of the process F strongly depend on the behaviour of G close to the ground state and may also display long-range correlations. To understand this point, consider the example in which $G^{a,b}(\omega) = \gamma$. This choice yields a spectral density of $F(t)$ which is logarithmically divergent close to the ground state frequency, thus defining a non-stationary process. The simplest, nonsingular case is obtained by choosing

$$G^a(\omega) = \frac{\gamma}{2\pi}(\omega - \mu), \quad G^b(\omega) = \frac{\gamma}{2\pi}(\omega + \mu) \quad .$$

In this case $F(t)$ becomes a complex white noise

$$\langle F(t)F^*(t') \rangle = \frac{\gamma}{\beta} \delta(t - t') \quad ,$$

while the dissipation function is

$$G(t) = \frac{\gamma}{2\pi} \int_{-\infty}^{+\infty} d\omega (\omega - \mu) e^{i\omega t} = -\gamma \left[i \frac{d}{dt} \delta(t) + \mu \delta(t) \right] \quad . \quad (37)$$

The full dissipation term is therefore

$$-i \int_0^t G(t-s)z(s) ds = -\gamma \dot{z}(t) + i\gamma\mu z(t) \quad , \quad (38)$$

and the resulting Langevin equation corresponds to a noisy, driven, complex Ginzburg-Landau equation

$$(i + \gamma)\dot{z} = f(z) + i\gamma\mu z + F(t) \quad . \quad (39)$$

In the weak coupling limit ($\gamma \ll 1$), the equation can be further simplified. By multiplying by $(1 + i\gamma)$ and neglecting terms $O(\gamma^{3/2})$, one obtains

$$i\dot{z} = (1 + i\gamma)f(z) + i\gamma\mu z + F(t) \quad , \quad (40)$$

which has the same structure as Eq. (5).

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